

Speaker: Peter W Kenny

Title: Accident and misadventure in property-based molecular design

Abstract: Following some general comments on property-based molecular design, I will show how trends in data can be exaggerated by hiding or masking variation. I will then discuss the deficiencies of ligand efficiency metrics (LEMs) which are widely used by drug discovery scientists to normalize affinity and biological activity with respect to pharmaceutical risk factors such as molecular size and lipophilicity. It will be argued that the trend actually observed in data sets should be used to normalize them and alternatives to LEMs for normalizing data will be presented.